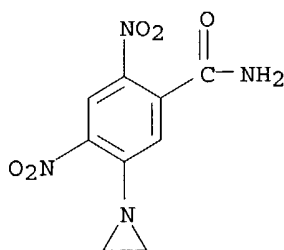


L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 21919-05-1 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN Benzamide, 5-(1-aziridinyl)-2,4-dinitro- (8CI, 9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN 2,4-Dinitro-5-ethyleneiminobenzamide  
 CN 2,4-Dinitroethyleneiminobenzamide  
 CN 5-(1-Aziridinyl)-2,4-dinitrobenzamide  
 CN 5-Aziridino-2,4-dinitrobenzamide  
 CN 5-Aziridinyl-2,4-dinitrobenzamide  
 CN **CB 1954**  
 CN NSC 115829  
 MF C9 H8 N4 O5  
 LC STN Files: ADISNEWS, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS,  
 BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CHEMCATS, CIN, DDFU, DRUGU,  
 EMBASE, IMSDRUGNEWS, IMSRESEARCH, MEDLINE, PROMT, PROUSDDR, RTECS\*,  
 TOXCENTER, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)  
 DT.CA Caplus document type: Conference; Dissertation; Journal; Patent  
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);  
 PROC (Process); RACT (Reactant or reagent); USES (Uses)  
 RLD.P Roles for non-specific derivatives from patents: BIOL (Biological  
 study); USES (Uses)  
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological  
 study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP  
 (Properties); RACT (Reactant or reagent); USES (Uses)  
 RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological  
 study); PRP (Properties)

#### Ring System Data

| Elemental<br>Analysis<br>EA | Elemental<br>Sequence<br>ES | Size of<br>the Rings<br>SZ | Ring System<br>Formula<br>RF | Ring<br>Identifier<br>RID | RID<br>Occurrence<br>Count |
|-----------------------------|-----------------------------|----------------------------|------------------------------|---------------------------|----------------------------|
| C2N                         | NC2                         | 3                          | C2N                          | 1.28.1                    | 1                          |
| C6                          | C6                          | 6                          | C6                           | 46.150.18                 | 1                          |



#### Calculated Properties (CALC)

| PROPERTY (CODE)       | VALUE | CONDITION | NOTE    |
|-----------------------|-------|-----------|---------|
| Bioconc. Factor (BCF) | 5.50  | pH 1      | (1) ACD |
| Bioconc. Factor (BCF) | 5.50  | pH 4      | (1) ACD |
| Bioconc. Factor (BCF) | 5.50  | pH 7      | (1) ACD |
| Bioconc. Factor (BCF) | 5.50  | pH 8      | (1) ACD |

|                            |                    |            |         |
|----------------------------|--------------------|------------|---------|
| Bioconc. Factor (BCF)      | 5.50               | pH 10      | (1) ACD |
| Boiling Point (BP)         | 427.2+/-45.0 deg C | 760.0 Torr | (1) ACD |
| Enthalpy of Vap. (Hvap)    | 68.22+/-3.0 kJ/mol |            | (1) ACD |
| Flash Point (FP)           | 212.2+/-51.7 deg C |            | (1) ACD |
| H acceptors (HAC)          | 9                  |            | (1) ACD |
| H donors (HD)              | 2                  |            | (1) ACD |
| Koc (KOC)                  | 118                | pH 1       | (1) ACD |
| Koc (KOC)                  | 118                | pH 4       | (1) ACD |
| Koc (KOC)                  | 118                | pH 7       | (1) ACD |
| Koc (KOC)                  | 118                | pH 8       | (1) ACD |
| Koc (KOC)                  | 118                | pH 10      | (1) ACD |
| logD (LOGD)                | 1.28               | pH 1       | (1) ACD |
| logD (LOGD)                | 1.28               | pH 4       | (1) ACD |
| logD (LOGD)                | 1.28               | pH 7       | (1) ACD |
| logD (LOGD)                | 1.28               | pH 8       | (1) ACD |
| logD (LOGD)                | 1.28               | pH 10      | (1) ACD |
| logP (LOGP)                | 1.277+/-0.423      |            | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L        | pH 1       | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L        | pH 4       | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L        | pH 7       | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L        | pH 8       | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L        | pH 10      | (1) ACD |
| Molecular Weight (MW)      | 252.18             |            | (1) ACD |
| Vapor Pressure (VP)        | 1.66E-07 Torr      | 25.0 deg C | (1) ACD |

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.67 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.  
153 REFERENCES IN FILE CA (1907 TO DATE)  
4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
153 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Sto.

FILE 'REGISTRY' ENTERED AT 09:28:57 ON 13 JUL 2004

E "5-(AZIRIDIN-1-YL)-2,4-DINITROBENZAMIDE"/CN 25

E "CB1954"/CN 25

E "CB 1954"/CN 25

L1 1 S E3

FILE 'CAPLUS' ENTERED AT 09:31:33 ON 13 JUL 2004

L2 151 S 21919-05-1/RN

L3 3 S L2 AND COSUBSTRATE

FILE 'STNGUIDE' ENTERED AT 09:33:25 ON 13 JUL 2004

FILE 'BIOSIS' ENTERED AT 09:42:13 ON 13 JUL 2004

L4 24 S CB 1954/CN

L5 0 S L4 AND COSUBSTRATE

L6 0 S L4 AND DIHYDROPYRIDINE

L7 0 S L4 AND NAH

L8 0 S L4 AND NRH

FILE 'PCTFULL' ENTERED AT 09:43:44 ON 13 JUL 2004

L9 0 S 21919-05-1/RN

L10 0 S CB 1954/CN

L11 44 S CB1954

L12 3 S L11 AND NRH

## WEST Search History

DATE: Tuesday, July 13, 2004

| <u>Hide?</u>             | <u>Set Name</u>                           | <u>Query</u>                   | <u>Hit Count</u> |
|--------------------------|---|--------------------------------|------------------|
|                          | <i>DB=PGPB,USPT,EPAB; PLUR=YES; OP=OR</i> |                                |                  |
| <input type="checkbox"/> | L13                                       | L11 and nicotinamide           | 10               |
| <input type="checkbox"/> | L12                                       | L11 not @py>2000               | 10               |
| <input type="checkbox"/> | L11                                       | L10 and l7                     | 29               |
| <input type="checkbox"/> | L10                                       | CB adj 1954                    | 37               |
| <input type="checkbox"/> | L9  | l7 and L8                      | 5                |
| <input type="checkbox"/> | L8  | NQO2                           | 21               |
| <input type="checkbox"/> | L7  | prodrugs                       | 19530            |
| <input type="checkbox"/> | L6  | l5 and l3                      | 3                |
| <input type="checkbox"/> | L5  | bioactivation                  | 310              |
| <input type="checkbox"/> | L4  | bioactivation                  | 1                |
| <input type="checkbox"/> | L3  | l1 with (analog or derivative) | 778              |
| <input type="checkbox"/> | L2  | nicotinamide with analogs      | 255              |
| <input type="checkbox"/> | L1  | nicotinamide                   | 6949             |

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**Web** Results **11 - 17** of about **21** for **NRH OR "dihydronicotinamide riboside OR "nicotinamide riboside** . (0

### Function GO Term Classification

... **dihydronicotinamide riboside** quinone reductase activity;  
 dihydropterin oxidase activity; ... L-ascorbate transporter activity;  
**nicotinamide** mononucleotide transporter ...  
[contact14.ics.uci.edu/fgo/function\\_class\\_3.html](http://contact14.ics.uci.edu/fgo/function_class_3.html) - 33k -  
[Cached](#) - [Similar pages](#)

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#### Nicotinamide

Yahoo! Shopping: Compare and Save.  
 Top brands, great stores, low price  
 Yahoo.com

### JBC -- Long et al. 277 (48): 46131

[See your message here...](#)

... NQO2 uses **dihydronicotinamide riboside** (NRH) rather than NAD(P)H as ... NRH was  
 synthesized by adding 1,000 units of ... l of 10 mM **nicotinamide** mononucleotide (Sigma ...

[www.jbc.org/cgi/content/full/277/48/46131](http://www.jbc.org/cgi/content/full/277/48/46131) - [Similar pages](#)

### [PDF] Disruption of Dihydronicotinamide Riboside:Quinone Oxidoreductase ...

File Format: PDF/Adobe Acrobat

... SP4 0JQ, United Kingdom **Dihydronicotinamide riboside** (NRH):quinone oxi ... NRH  
 was synthesized by adding 1,000 units of ... of 10 m M **nicotinamide** mononucleotide  
 (Sigma ...

[www.jbc.org/cgi/reprint/277/48/46131.pdf](http://www.jbc.org/cgi/reprint/277/48/46131.pdf) - Supplemental Result - [Similar pages](#)

### PNAS -- Zhao et al. 94 (5): 1669

... ionization mass spectrometry; NMNH, reduced **nicotinamide** mononucleotide; QR 1 ...  
 and AK Jaiswal Disruption of **Dihydronicotinamide Riboside**:Quinone Oxidoreductase ...  
[www.pnas.org/cgi/content/full/94/5/1669](http://www.pnas.org/cgi/content/full/94/5/1669) - [Similar pages](#)

### Bioactivation of 5-(aziridin-1-yl)-2,4-dinitrobenzamide (CB 1954) ...

... NQO2 [NAD(P)H quinone oxidoreductase 2], but its activity is normally latent, and a  
 nonbiogenic co-substrate such as NRH [**nicotinamide riboside** (reduced)] is ...

[www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&](http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=PubMed&list_uids=10945627&dopt=Citation)

[db=PubMed&list\\_uids=10945627&dopt=Citation](#) - Supplemental Result - [Similar pages](#)

### DISEOME

... M:Receptors, Muscarinic **nicotinamide** histochemistry muscarinic ... derived nondeletion  
**NRH** detoxified GGGCGGG GSTM1-positive **riboside** gene-environment ...

[www.snps3d.org/cgi-bin/tg/index.pl?key=1728&type=geneShell](http://www.snps3d.org/cgi-bin/tg/index.pl?key=1728&type=geneShell) - 101k - Supplemental  
 Result - [Cached](#) - [Similar pages](#)

### keywords shared by GSTA2 and NQO1 GSTM1 butyl carcinogens oxidant ...

... alleles of the human reduced **nicotinamide** adenine dinucleotide ... H:quinone  
 oxidoreductase 1 (NQO1) and **dihydronicotinamide riboside** (NRH):quinone  
 oxidoreductase ...

[www.snps3d.org/cgi-bin/tg/edge.pl?n1=2939&n2=1728](http://www.snps3d.org/cgi-bin/tg/edge.pl?n1=2939&n2=1728) - 56k - Supplemental Result -  
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